2,2-Dimethyl-1,3-dioxolane
2916-31-6 | DTXSID10183419

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.76

Global applicability domain: Inside

Local applicability domain index: 5.62e-01

Confidence level: 6.30e-01

Nearest Neighbors from the Training Set

Image not found
4-Methylimidazolidine-2-thione
Measured: 10.0
Predicted: 4.59

Image not found
1,4-Dioxane
Measured: 5.01e-01
Predicted: 1.06

Image not found
Diethyl ether
Measured: 5.37
Predicted: 4.72

Image not found
2-Aminopyridine
Measured: 11.5
Predicted: 3.44

Image not found
3-Pyridinamine
Measured: 2.09
Predicted: 3.04